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13. SUPPLEMENTARY NOTES

14. ABSTRACT

In this project we have investigated the use of global optimization techniques for device design problem in photonics and electronics. Using several concrete device design problems as guides, we have defined a sub-class of global optimization problems with high-dimensional design space as the main focus of our effort. We have evaluated optimization approaches including Genetic Algorithm and Simulated Annealing for this class of problems. This evaluation confirmed our previous experience in using these techniques in global optimal design problem. In fact these methods do not effectively use all available local information during the search for the global optimal solution and can easily be trapped near locally optimal solutions. We have subsequently developed an Ensemble Global Optimization (EnGO) technique that explicitly defines region of exclusions around already examined points in the design space to allow maximal coverage of the design space through randomized search. At the same time local gradient information is used to accelerate convergence to local and global optimal solution. The method is being tested successfully on prototype problems in relatively high dimensional design space.

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Final Report for the Project

Ensemble Techniques for Determining Globally Optimal Designs for Problems with Broadly Stated Design Objectives

1. Purpose of the Project

Problems in design of advanced photonic and electronic devices often require the search over high-dimensional design spaces to optimize highly non-convex performance functions. The large number of design parameters is also making it extremely difficult to rely on intuition of design engineers to develop near-optimal candidate designs. As a result, local optimization techniques are not sufficient for these problems. Prior to the start of this project, the main investigators have experimented with other commonly used global optimization approaches including Genetic Algorithm (GA) and Simulated Annealing (SA). However, these techniques tend to not make use of all available local information such as the gradient and approximated Hessian of the performance function. On the other hand, the existing techniques rely on analogies with natural evolution or random motion of energize particle to bias the exploration of the design space. Unfortunately, these analogies are often non-intuitive for optimal design problems. The primary purpose of this project is to make use of the basic ideas of ensemble technique to develop an alternative global optimization technique for global optimal design problems. The ensemble technique has been successfully used in weather forecasting and large scale data assimilation. The key idea of ensemble technique is to use parallel evaluations of a highly complex system model over a variety of conditions to obtain valuable information on the system. The new algorithm is designed to solve optimization problems for which the evaluation of the performance functional is very computationally intensive and the design space is a compact subset of a high-dimensional vector space. Since for many design problems it is also interesting to identify locally optimal but globally sub-optimal design solutions, the new algorithm needs to efficiently distribute ensemble members to provide as complete coverage of the entire design space as possible and identify locally optimal designs in the exploration process.

2. Major Achievement of the Project

In the short period of the performance of this project, we have developed and implemented an Ensemble Global Optimization (EnGO) technique that allow hierarchical random search of the design space with progressively finer coverage and, at the same time, effectively use available local gradient information to accelerate convergence to locally and globally optimal solutions. The exploration of the design space through an ensemble of candidate designs enables the algorithm to quickly abandon a non-promising candidate when the relative performance of the candidate design is inferior to other candidates. Multiple ensemble statistical criteria are used to eliminate redundant search of the same area of the design space and to minimize exploration around non promising regions of the design space.

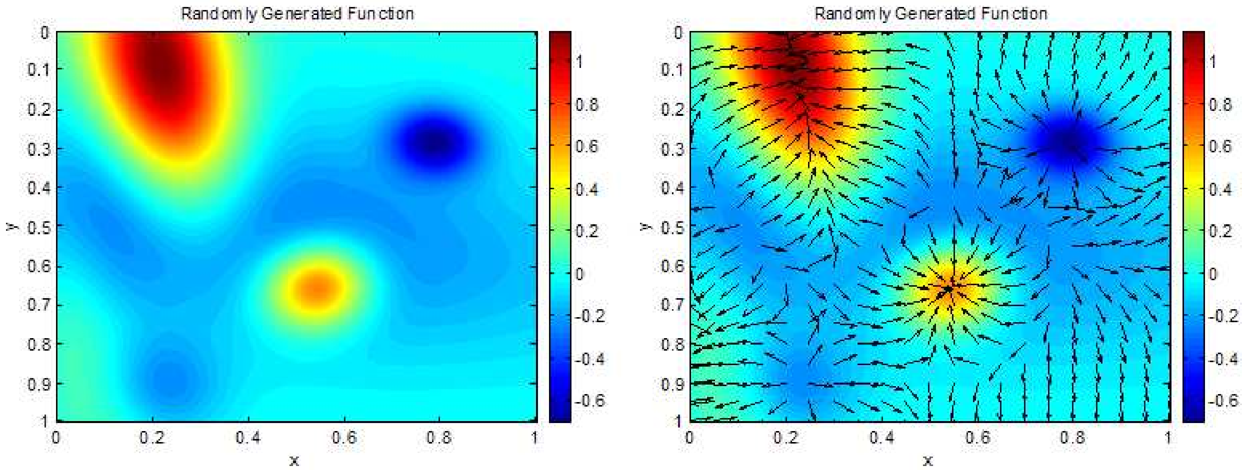
In addition to the development of the EnGO, we have developed a systematic method to evaluate the performance of a global optimization method on a class of randomly generated functions in high dimensional vector spaces. This methodology provides us with a test-bed to evaluate and improve EnGO. The class of the randomly generated functions has the form

$$J(\vec{x}) = \sum_{k=1}^{n} a_k \cdot \exp\left(-\left(\vec{x}-\vec{s}_k\right)^T A_k^{-1}\left(\vec{x}-\vec{s}_k\right)\right).$$

The quantities a_k, A_k and $\vec{s}_k$ are randomly generated values, covariant matrices and vectors, respectively. For each value of *k*, the component of the function reaches either maximum or minimum at the seed point $\vec{s}_k$. The function trends to zeros at infinity. The selection of this class of random functions meets the following criteria important for device design problems:

- The performance function is locally smooth function of the design variables and the gradient of performance function can be efficiently evaluate;
- There is a small neighborhood around the globally and locally optimal design such that when a gradient based local optimization algorithm starts with an initial solution inside of this neighborhood, the algorithm converges toward the optimal design, and
- The function is computationally easy to evaluate to be used for testing of global optimization scheme.

An example of a random function in 2-dimensional space is given shown in Figure 1.



(a) (b)

Figure 1. 2-dimensional randomly generated function (a) and its gradient field (b)

We have evaluated EnGO against GA and SA using this class of functions. An example of the result in 5D is shown in Figure 2 and 3.

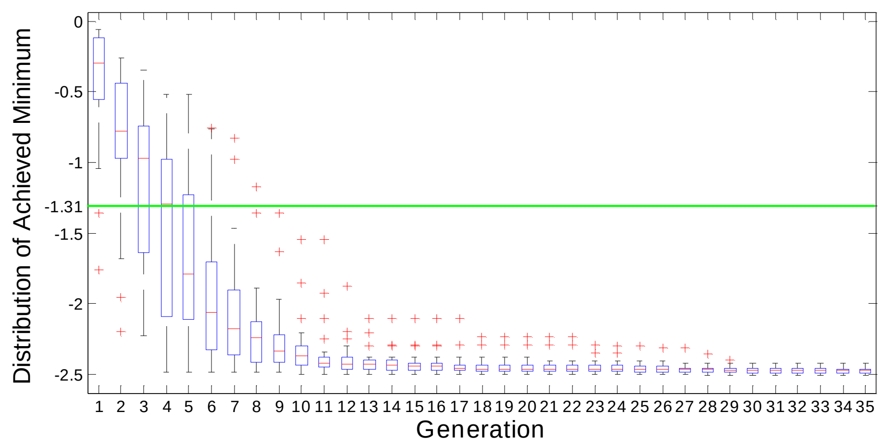


Figure 2. Performance of EnGO for 5D

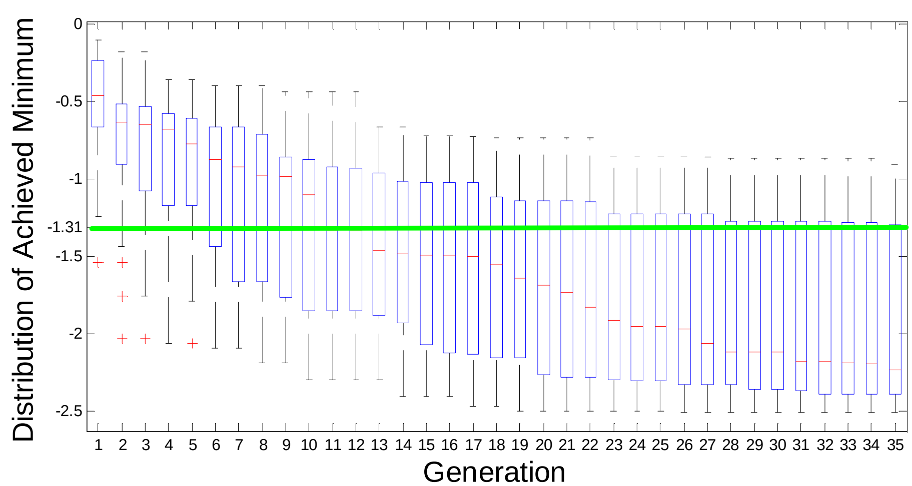


Figure 3. Performance of GA

Since both EnGO and GA use random generation of candidate designs in the search process, it is important to evaluate these algorithms in statistically meaningful way. In our evaluation, each of the algorithms is evaluated over 30 repeated test runs on the same underlying function. In each test run, 20 ensemble members are used and 35 iterations are performed. In Figure 2 and 3, the statistics of the 30 minimal values among the 20 ensemble members for each of the test runs are displayed. After 35 generations, a substantial portion of the test runs for GA is trapped at a local minimum in the design space while the EnGO algorithm is successful in all test runs to find the global minimum of the problem.

An important challenge in high-dimensional global optimization is the “curse of dimensionality”. That is the volume of space to explore increases exponentially. We have developed strategy to work in high-dimensional problems. In fact, we have successfully tested our approach for a 10-dimensional problem as shown in Figure 4.

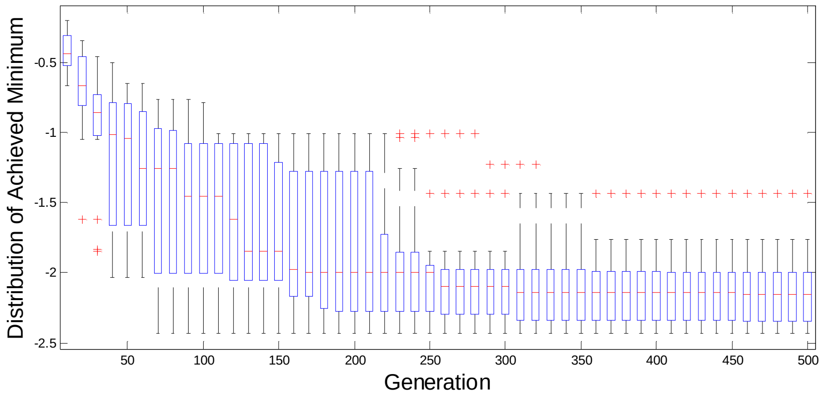


Figure 4. Test results for EnGO on a 10-dimensional problem

Future Research

Our immediate next step is to implement the EnGO for two prototype design problems in electromagnetic device design and electronic device design. This will allow us to demonstrate the potential of the EnGO in contributing to the improvement over local optimization based design approaches.

Parallel to the application of EnGO on the prototype problems, we are continuing the development of EnGO in better handling of high-dimensional design problem and multiple objective design problems.